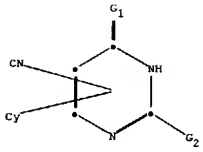
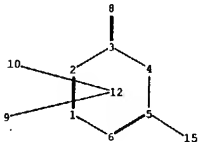
C:\Program Files\Stnexp\Queries\10799507



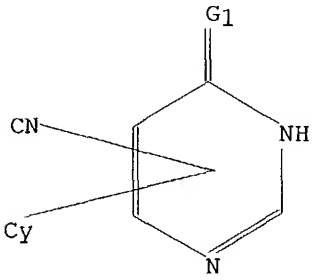

chain nodes :
8 9 10 15
ring nodes :
1 2 3 4 5 6
chain bonds :
3-8 5-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-8 4-5 5-6 5-15
isolated ring systems :
containing 1 :

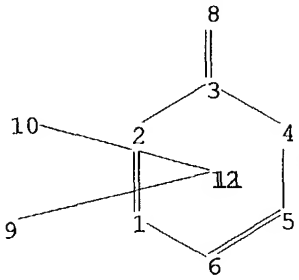
G1:O,S

G2:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS

=>
Uploading C:\Program Files\Stnexp\Queries\10799507.str



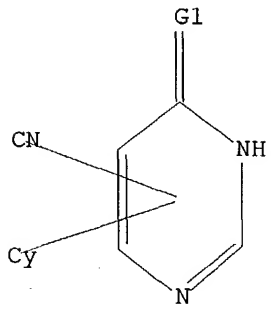

chain nodes :
8 9 10
ring nodes :
1 2 3 4 5 6
chain bonds :
3-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-8 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS 11:CLASS
12:CLASS

L1 STRUCTURE UPLOADED

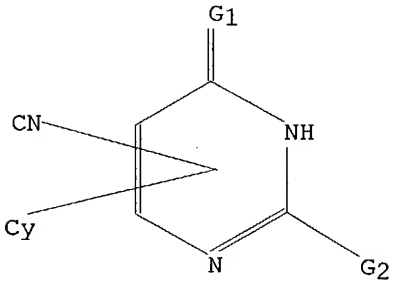
=> d l1
L1 HAS NO ANSWERS
L1 STR

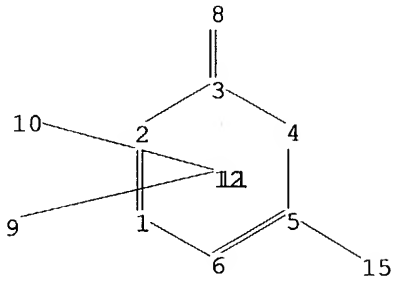



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

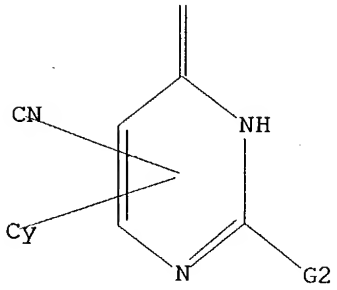
```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 19:05:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1471 TO ITERATE

 68.0% PROCESSED    1000 ITERATIONS                                  30 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         27120 TO    31720
PROJECTED ANSWERS:              484 TO     1280

L2            30 SEA SSS SAM L1

=> =>
Uploading C:\Program Files\Stnexp\Queries\10799507 (a).str
```




```
chain nodes :
8  9  10  15
ring nodes :
1  2  3  4  5  6
chain bonds :
3-8  5-15
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  3-8  4-5  5-6  5-15
isolated ring systems :
containing 1 :


G1:O,S

G2:H,CH3

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:Atom  10:CLASS  11:CLASS
 12:CLASS  15:CLASS



L3      STRUCTURE UPLOADED

=> d l3
```

L3 HAS NO ANSWERS
L3 STR




G1 O,S
G2 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l3 sss sam
SAMPLE SEARCH INITIATED 19:08:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1471 TO ITERATE

68.0% PROCESSED 1000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 27120 TO 31720
PROJECTED ANSWERS: 2 TO 160

L4 2 SEA SSS SAM L3

=> s l3 sss ful
FULL SEARCH INITIATED 19:08:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 30608 TO ITERATE

100.0% PROCESSED 30608 ITERATIONS 85 ANSWERS
SEARCH TIME: 00.00.01

L5 85 SEA SSS FUL L3

=> => s l5
L6 19 L5

=> d l6 1-19 bib,ab,hitstr

L6 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:780676 CAPLUS
TI Preparation of 4-substituted-5-cyano-1H-pyrimidin-6-(thi)ones as glycogen synthase kinase-3 (GSK-3) inhibitors.
IN Moon, Young-Choon
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DT Patent
LA English

Appl PCT

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2004080977 | A1 | 20040923 | WO 2004-US7801 | 20040312 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2004186119 | A1 | 20040923 | US 2004-799507 | 20040312 |
| PRAI US 2003-454878P | P | 20030312 | | |

AB Title compds. [I; W = O, S; A = 5-6 membered aryl, heteroaryl optionally substituted by halo, cyano, OR1, N(R1)2, NR1NR1CON(R1)2, NR1COR1, COCOR1, COR1, SO2R1, NR1CO2R1, CO2R1, O, S, NR1, etc.; R1 = H, (substituted) aliphatyl, aryl, heteroaryl, heterocyclyl], are claimed (no synthetic or biol. data).

IT **543700-28-3P 760966-32-3P 760966-33-4P**
**760966-34-5P 760966-35-6P 760966-36-7P**
**760966-37-8P 760966-38-9P 760966-39-0P**
**760966-40-3P 760966-41-4P 760966-42-5P**
**760966-43-6P 760966-44-7P 760966-45-8P**
**760966-46-9P 760966-47-0P 760966-48-1P**
**760966-49-2P 760966-50-5P 760966-51-6P**
**760966-52-7P 760966-53-8P 760966-54-9P**
**760966-55-0P 760966-56-1P 760966-57-2P**
**760966-58-3P 760966-59-4P 760966-60-7P**
**760966-61-8P 760966-62-9P 760966-63-0P**
**760966-64-1P 760966-65-2P 760966-66-3P**
**760966-67-4P 760966-68-5P 760966-69-6P**
**760966-70-9P 760966-71-0P 760966-72-1P**
**760966-73-2P 760966-74-3P 760966-75-4P**
**760966-76-5P 760966-77-6P 760966-78-7P**
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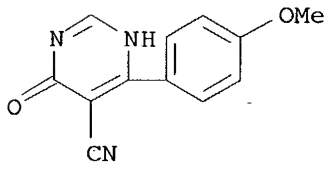
**760966-82-3P 760966-83-4P 760966-84-5P**
**760966-85-6P 760966-86-7P 760966-87-8P**
**760966-88-9P 760966-89-0P 760966-90-3P**
**760966-91-4P 760966-92-5P 760966-93-6P**
**760966-94-7P 760966-95-8P 760966-96-9P**
**760966-97-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of substituted cyanopyrimidinones as glycogen synthase kinase-3 inhibitors)

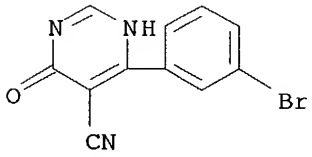
RN 543700-28-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



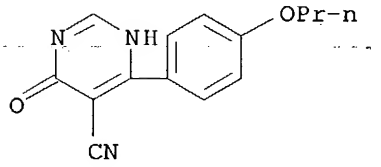

RN 760966-32-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 6-(3-bromophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



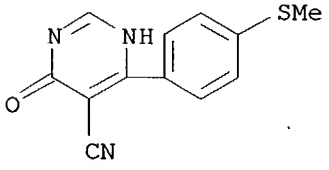

RN 760966-33-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(4-propoxyphenyl)- (9CI) (CA INDEX NAME)



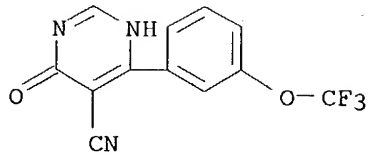

RN 760966-34-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-[4-(methylthio)phenyl]-4-oxo- (9CI) (CA INDEX NAME)

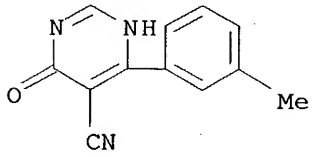



RN 760966-35-6 CAPLUS

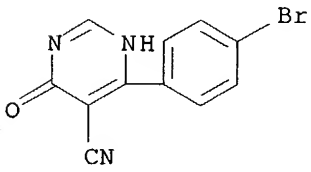
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-[3-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



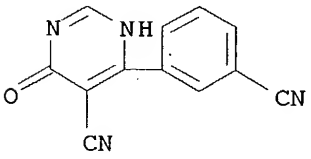
RN 760966-36-7 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(3-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)



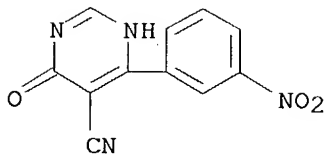
RN 760966-37-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(4-bromophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



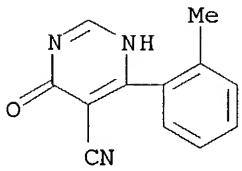
RN 760966-38-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-cyanophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



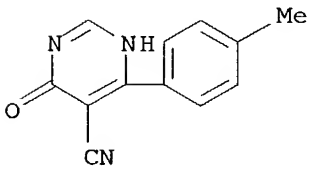
RN 760966-39-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(3-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)



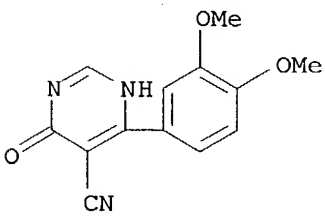
RN 760966-40-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(2-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)



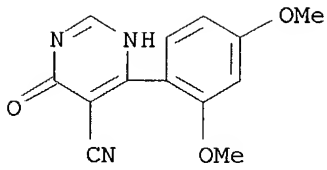
RN 760966-41-4 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)



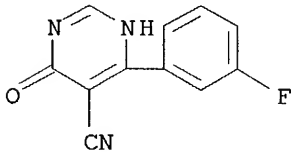
RN 760966-42-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3,4-dimethoxyphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



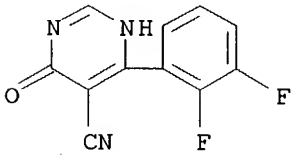
RN 760966-43-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2,4-dimethoxyphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



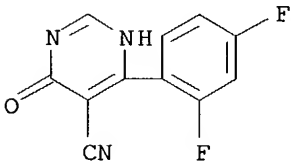
RN 760966-44-7 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-fluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



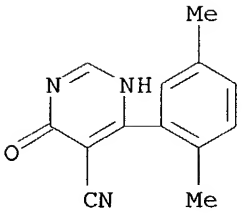
RN 760966-45-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2,3-difluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



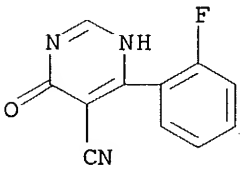
RN 760966-46-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2,4-difluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



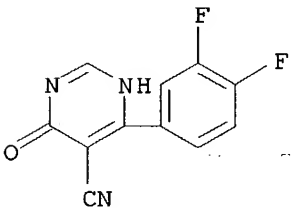
RN 760966-47-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2,5-dimethylphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



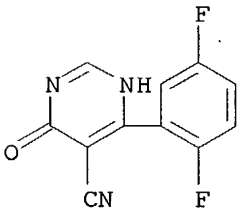
RN 760966-48-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2-fluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



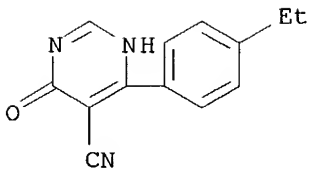
RN 760966-49-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3,4-difluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



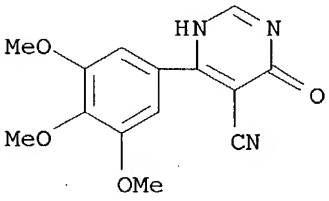
RN 760966-50-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(2,5-difluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



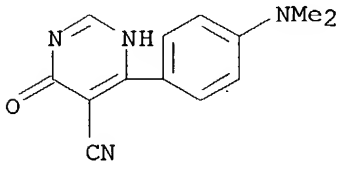
RN 760966-51-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(4-ethylphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



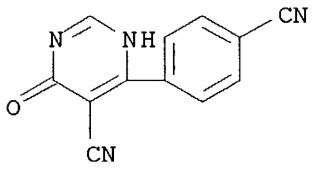
RN 760966-52-7 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



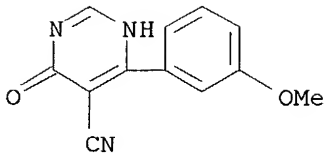
RN 760966-53-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-[4-(dimethylamino)phenyl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



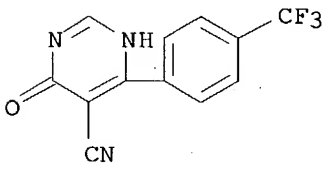
RN 760966-54-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(4-cyanophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



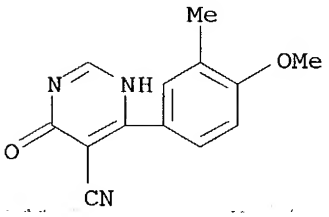
RN 760966-55-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(3-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



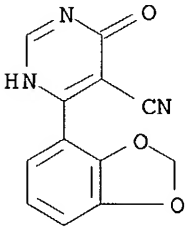
RN 760966-56-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-[4-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)



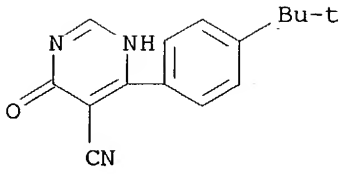
RN 760966-57-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxy-3-methylphenyl)-4-oxo-(9CI) (CA INDEX NAME)



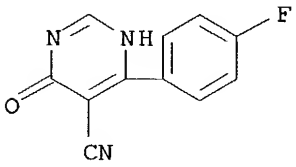
RN 760966-58-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



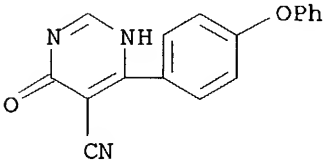
RN 760966-59-4 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-[4-(1,1-dimethylethyl)phenyl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



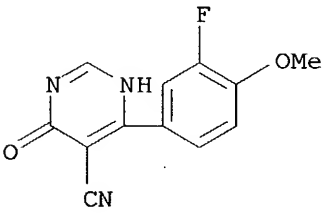

RN 760966-60-7 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(4-fluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



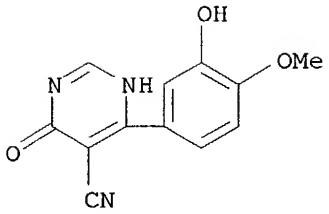

RN 760966-61-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)



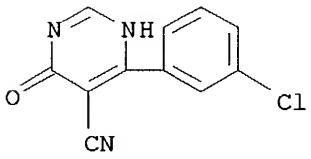

RN 760966-62-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



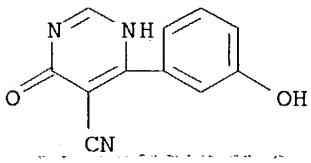

RN 760966-63-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(3-hydroxy-4-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



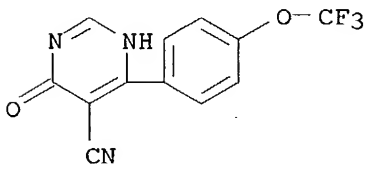
RN 760966-64-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-chlorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



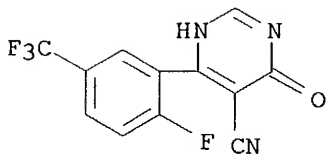
RN 760966-65-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(3-hydroxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



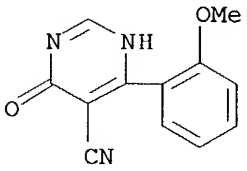
RN 760966-66-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



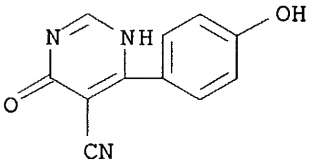
RN 760966-67-4 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-[2-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



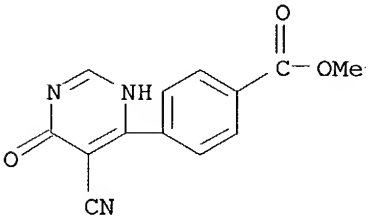
RN 760966-68-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(2-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



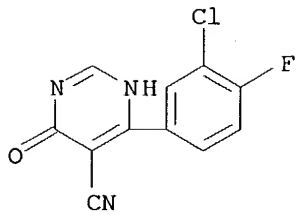
RN 760966-69-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-hydroxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



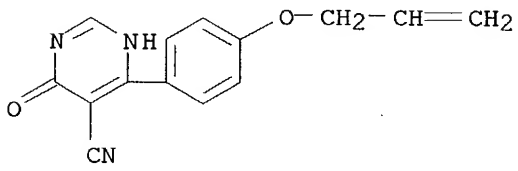
RN 760966-70-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



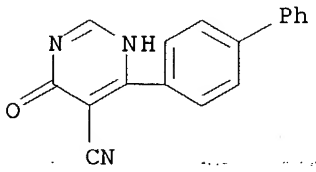
RN 760966-71-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



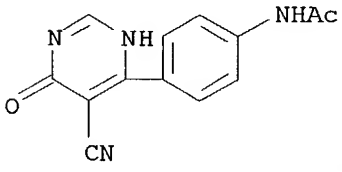
RN 760966-72-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-[4-(2-propenyloxy)phenyl]- (9CI) (CA INDEX NAME)



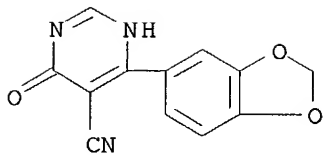
RN 760966-73-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-[1,1'-biphenyl]-4-yl-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



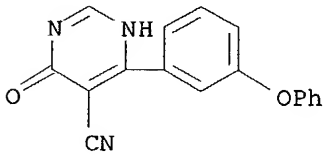
RN 760966-74-3 CAPLUS
CN Acetamide, N-[4-(5-cyano-1,6-dihydro-6-oxo-4-pyrimidinyl)phenyl]- (9CI) (CA INDEX NAME)



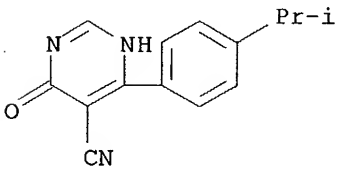
RN 760966-75-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



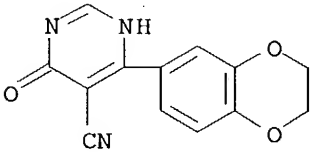
RN 760966-76-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(3-phenoxyphenyl)- (9CI) (CA INDEX NAME)



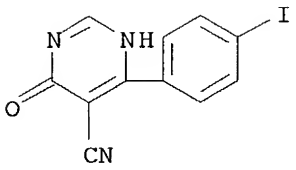
RN 760966-77-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-[4-(1-methylethyl)phenyl]-4-oxo- (9CI) (CA INDEX NAME)



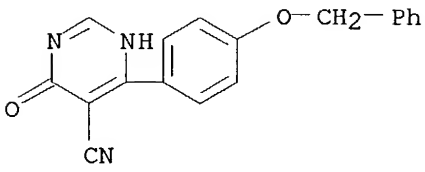
RN 760966-78-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



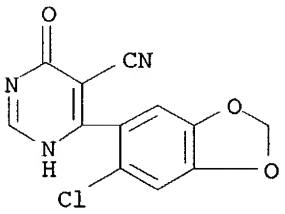
RN 760966-79-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-iodophenyl)-4-oxo- (9CI) (CA INDEX NAME)



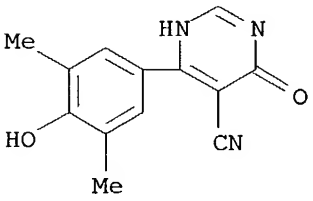
RN 760966-80-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



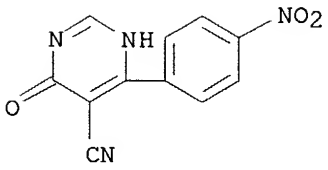
RN 760966-81-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



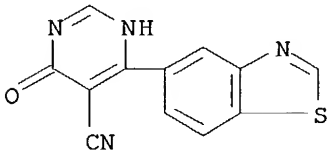
RN 760966-82-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-hydroxy-3,5-dimethylphenyl)-4-oxo- (9CI) (CA INDEX NAME)



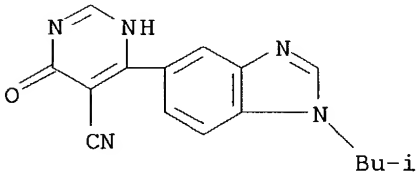
RN 760966-83-4 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)



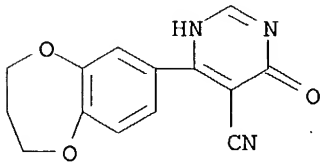
RN 760966-84-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(5-benzothiazolyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



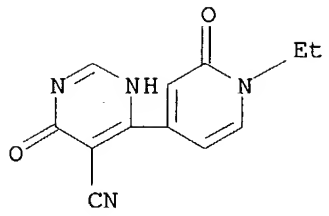
RN 760966-85-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-[1-(2-methylpropyl)-1H-benzimidazol-5-yl]-4-oxo- (9CI) (CA INDEX NAME)



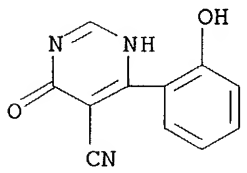
RN 760966-86-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



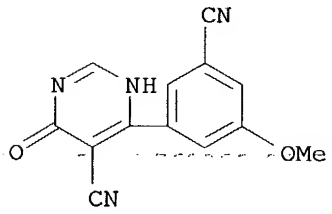
RN 760966-87-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(1-ethyl-1,2-dihydro-2-oxo-4-pyridinyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



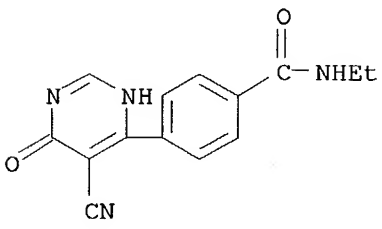
RN 760966-88-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(2-hydroxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



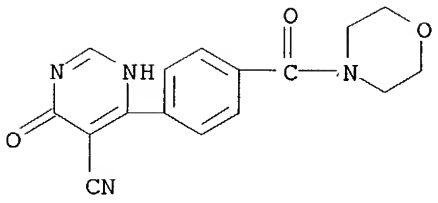
RN 760966-89-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-cyano-5-methoxyphenyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



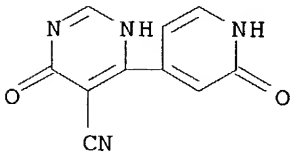
RN 760966-90-3 CAPLUS
CN Benzamide, 4-(5-cyano-1,6-dihydro-6-oxo-4-pyrimidinyl)-N-ethyl- (9CI) (CA INDEX NAME)



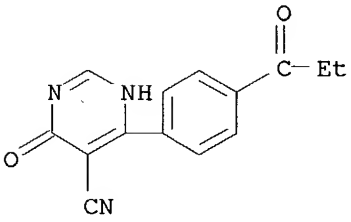
RN 760966-91-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



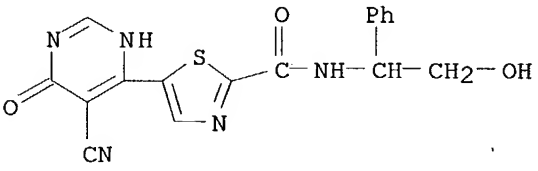
RN 760966-92-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(1,2-dihydro-2-oxo-4-pyridinyl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



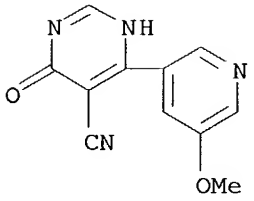
RN 760966-93-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



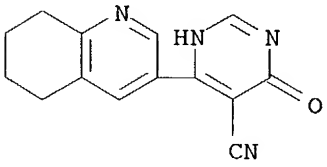
RN 760966-94-7 CAPLUS
CN 2-Thiazolecarboxamide, 5-(5-cyano-1,6-dihydro-6-oxo-4-pyrimidinyl)-N-(2-hydroxy-1-phenylethyl)- (9CI) (CA INDEX NAME)



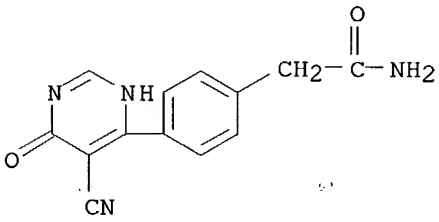
RN 760966-95-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(5-methoxy-3-pyridinyl)-4-oxo- (9CI) (CA INDEX NAME)



RN 760966-96-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(5,6,7,8-tetrahydro-3-quinolinyl)- (9CI) (CA INDEX NAME)

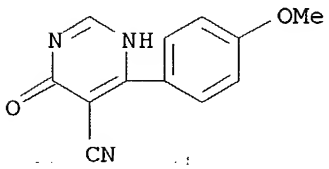


RN 760966-97-0 CAPLUS
CN Benzeneacetamide, 4-(5-cyano-1,6-dihydro-6-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:190837 CAPLUS
DN 139:36510
TI Synthesis of bioactive aza-heterocyclic systems derived from novel biheterocyclic enone
AU Abdel-Megid, M.; Ismail, M. M.
CS Chemistry Department, Faculty of Education, Ain-Shams University, Cairo, Egypt
SO International Journal of Chemistry (2002), 12(4), 287-296
CODEN: INJCEW
PB Institute of Science & Technology
DT Journal
LA English
OS CASREACT 139:36510
AB Some interesting bioactive Aza-heterocycles bearing quinolinone and pyridazinone moieties, such as pyrazoles, isoxazole, cyanopyridinethione pyrimidinethione, pyrimidopyrimidine, thiazines, diazepines, oxazepines and thiazepine have been synthesized from 1-(5,6-diphenyl-2-H-3-oxopyridazin-4-yl)-3-(1-ethyl-4-hydroxy-2- oxoquinolin-3-yl) propenone (I). Some of the newly products were subjected under biol. tests.
IT **543700-28-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of bioactive aza-heterocyclic systems derived from novel biheterocyclic enone)
RN 543700-28-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)

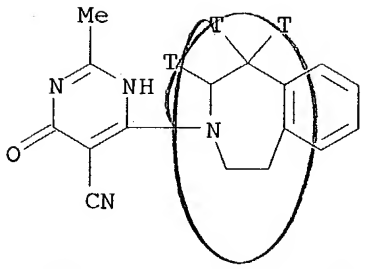



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:72103 CAPLUS
DN 136:134776
TI Preparation of tetrahydro-heterocycloazepinyl pyrimidines as mGluR antagonists
IN Binggeli, Alfred; Maerki, Hans-Peter; Mutel, Vincent; Wostl, Wolfgang; Wilhelm, Maurice
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2002006288 | A1 | 20020124 | WO 2001-EP8186 | 20010716 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | US 6369222 | B1 | 20020409 | US 2001-902916 | 20010711 |
| | US 2002045635 | A1 | 20020418 | | |
| | EP 1303521 | A1 | 20030423 | EP 2001-978247 | 20010716 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| | BR 2001012586 | A | 20030520 | BR 2001-12586 | 20010716 |
| | JP 2004504324 | T2 | 20040212 | JP 2002-512190 | 20010716 |
| PRAI | EP 2000-115450 | A | 20000718 | | |
| | WO 2001-EP8186 | W | 20010716 | | |

OS MARPAT 136:134776
AB The title compds. [I; R1 = O, OH, alkoxy, 2,2,2-trifluoroethoxy; R2 = NO2, CN; R3 = H, alkyl, alkoxy, etc.; R4 = H, alkyl, alkenyl or is absent; R5, R6, R9, R10 = H, alkyl; CR11R12HETCR7R8 = II-V; R7, R8, R11, R12 = H, alkyl, OH; R13, R14 = H, alkyl; R15, R16 = H, alkyl; R17 = H, alkyl, alkoxy, OH, NH2; R18 = H, OH; R19 = H, alkyl, alkoxy, OH, NH2; V = NH, S, O] which are mGluR antagonists and are therefore useful for the control or prevention of acute and/or chronic neurol. disorders, were prepared and formulated. Thus, reacting 6-bromo-2-methyl-5-nitro-3H-pyrimidin-4-one (preparation given) with 2-methyl-5,6,7,8-tetrahydro-4H-thiazolo[4,5-d]azepine.HCl in the presence of K2CO3 in DMF afforded 78.5% VI which showed IC50 of 30 μM against mGluR1 binding.
IT **391953-88-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrahydro-heterocycloazepinyl pyrimidines as mGluR antagonists)
RN 391953-88-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-4-oxo-6-(1,2,4,5-tetrahydro-1-t-3H-3-benzazepin-3-yl-1,2-t2)- (9CI) (CA INDEX NAME)

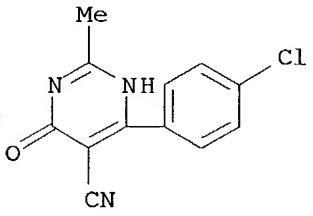



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:693290 CAPLUS
DN 135:257254
TI Preparation of pyrimidinone derivatives as herbicides or pesticides
IN Kudo, Yoshihiro; Katsumata, Akira; Maeda, Kazushige; Akiyama, Shigeaki; Yaosaka, Manabu; Morimoto, Katsushi; Nakahira, Kunimitsu; Ohki, Tooru; Hamada, Nobuyuki; Yano, Tetsuhiko; Noguchi, Junko; Watanabe, Shigeomi
PA Nissan Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 186 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2001068613 | A1 | 20010920 | WO 2001-JP2158 | 20010319 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | JP 2002220377 | A2 | 20020809 | JP 2001-76067 | 20010316 |
| PRAI | JP 2000-76493 | A | 20000317 | | |
| | JP 2000-357541 | A | 20001124 | | |

OS MARPAT 135:257254
AB Title compds. [I; R = H, CHF2, CH3, (CH3)2CH, CHCCH2, CH3SCH2, CH3SO2CH2, CH3OCH2, CH2F(CH2)2; Y = O, S; X = H, C1-4 alkyl; Z1 = N, CR1; R1 = H, Cl, CN, CHCCH2O; Z2 = CH, N; Q = aryl, benzoheterocycle] and salts are prepared as herbicides or pesticides. Thus, the title compound II was prepared and tested for herbicidal effect.
IT **361430-05-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinone derivs. as herbicides or pesticides)
RN 361430-05-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(4-chlorophenyl)-1,4-dihydro-2-methyl-4-oxo- (9CI) (CA INDEX NAME)




RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:98457 CAPLUS
DN 134:147611
TI Preparation of tetrahydrobenzo[d]azepines as metabotropic glutamate receptor 1 antagonists
IN Adam, Geo; Binggeli, Alfred; Maerki, Hans-Peter; Mutel, Vincent; Wilhelm, Maurice; Wostl, Wolfgang
PA F. Hoffmann-La Roche A.-G., Switz.
SO Eur. Pat. Appl., 85 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 1074549 | A2 | 20010207 | EP 2000-116091 | 20000727 |
| | EP 1074549 | A3 | 20020731 | | |
| | EP 1074549 | B1 | 20031119 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | AT 254614 | E | 20031215 | AT 2000-116091 | 20000727 |
| | CA 2314798 | AA | 20010206 | CA 2000-2314798 | 20000801 |
| | US 6218385 | B1 | 20010417 | US 2000-630702 | 20000801 |
| | NZ 506096 | A | 20020828 | NZ 2000-506096 | 20000801 |
| | ZA 2000003927 | A | 20010206 | ZA 2000-3927 | 20000802 |
| | AU 2000048979 | A5 | 20010208 | AU 2000-48979 | 20000802 |
| | AU 774485 | B2 | 20040701 | | |
| | HR 2000000520 | A1 | 20010630 | HR 2000-520 | 20000802 |
| | SG 93251 | A1 | 20021217 | SG 2000-4344 | 20000802 |
| | NO 2000003966 | A | 20010207 | NO 2000-3966 | 20000804 |
| | CN 1283623 | A | 20010214 | CN 2000-122523 | 20000804 |
| | TR 200002298 | A2 | 20010321 | TR 2000-200002298 | 20000804 |
| | JP 2001089472 | A2 | 20010403 | JP 2000-236848 | 20000804 |
| | JP 3260350 | B2 | 20020225 | | |
| | BR 2000003375 | A | 20010313 | BR 2000-3375 | 20000807 |
| PRAI | EP 1999-115557 | A | 19990806 | | |

OS MARPAT 134:147611
AB The title compds. (I) [wherein R1 = H, alkyl, O, halo, OR, cycloalkoxy, (un)substituted cycloalkylalkoxy, cyanoalkoxy, (fluoro)alkoxy, aminoalkoxy, alkenyloxy, phenylalkoxy, heterocyclylalkoxy, sulfonyloxyalkoxy, SR, carboxyalkylthio, NR2, hydroxyalkylamino, or heterocyclylalkylamino; n = 1-6; R = independently H, alkyl, or alkenyl; R2 = NO2 or CN; R3 = H, alkyl, O, S, SR, alkylsulfonyl, cycloalkyl, CONR2, NR2, alkyl, OR, or (un)substituted piperazino, carbamoylalkyl, alkoxyalkyl, fluoroalkyl, trifluoroacetoxyalkyl, carboxyalkyl, phenylthioalkyl, hetercyclylalkoxy, acylamino, alkylamino, phenoxyalkylamino, heterocyclylalkylamino, fluoroalkoxy, etc.; R4 = H, alkyl, alkenyl, NO2, OR, NR2, or (un)substituted fluoroalkoxy, fluoroalkyl, phenylalkyl, alkoxyalkanol, aminoalkyl, carboxyalkyl, alkylsulfonyloxyalkyl, fluoroalkenyl, heterocyclylalkyl, heterocyclylalkylamino, alkoxycarbonylamino, alkoxycarbonylhydrazino, aminofluoroalkenylamino; or R4 and R1 or R3 and R4 form an addnl. ring; R5 and R6 = independently H, alkyl, alkoxy, NH2, HO2, SO2NH2, or halo; or R5 and R6 = OCH2O; R7 and R8 = independently H, alkyl, alkoxy, NH2, NO2, or halo; R9 and R10 = independently H or alkyl; R11 and R12 = independently H, alkyl, OH, alkoxy, alkoxycarbonyloxy, or alkanoyloxy; R13 and R14 = independently H, T, or alkyl; R15 and R16 = independently H, T, alkyl, OH, alkoxy, alkoxycarbonyloxy, or alkanoyloxy; or R15 and R16 = O; X = N or C;

Y = N, NH, or CH] were prepared For example, addition of Et 2-cyano-3,3-bis(methylthio)acrylate to 2,3,4,5-tetrahydro-1H-benzo[d]azepine•HCl using TEA and K2CO3 in EtOH gave 2-cyano-3-methylsulfanyl-3-(1,2,4,5-tetrahydrobenzo[d]azepin-3-yl)acrylic acid Et ester (64%). The benzazepinylacrylate ester was treated with NH2C(NH)NH2•HNO3 and 1,8-diazabicyclo[5.4.0]undec-7-ene in DMF to give II (R = H). Ethylation of II (R = H) with EtI in DMF in the presence of K2CO3 afforded the preferred metabotropic glutamate receptor 1 (mGluR1) antagonist II (R = Et), which gave an IC50 values of 0.009 μM and 0.003 μM, resp. in functional and binding assays for the characterization of mGluR1 antagonist properties. I are useful in the prevention or control of acute and/or chronic neurol. disorders and as radiolabeled mGluR1 receptor antagonists in binding assays (no data).

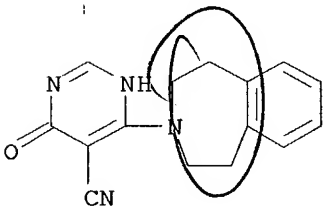
IT **324552-69-4P 324553-54-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of tetrahydrobenzo[d]azepine mGluR1 antagonists by addition of chloroheterocycles or halobenzenes to tetrahydrobenzo[d]azepines or by cycloaddn. of guanidines to 3-methylthio-3-(tetrahydrobenzo[d]azepin-3-yl)acrylates)

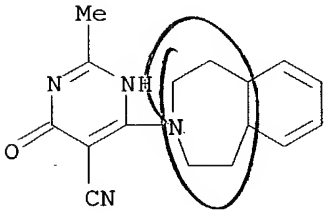
RN 324552-69-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-(1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl)- (9CI) (CA INDEX NAME)

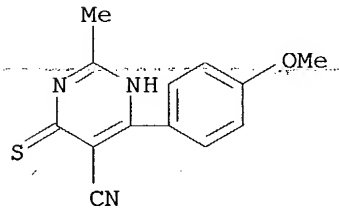



RN 324553-54-0 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-4-oxo-6-(1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl)- (9CI) (CA INDEX NAME)

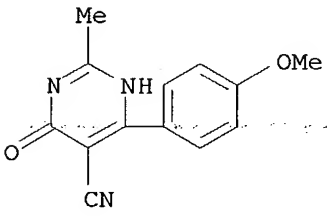


L6 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:256839 CAPLUS
DN 133:30702
TI Nitrogen bridgehead compounds, facile synthesis of bioactive cyanopyrimido[1,2-a]pyrimidinones
AU Abdel-Megid, Mohamed
CS Chemistry Department, Faculty of Education, Ain-Shams University, Cairo, Egypt
SO Pharmazie (2000), 55(4), 263-268
CODEN: PHARAT; ISSN: 0031-7144
PB Govi-Verlag Pharmazeutischer Verlag
DT Journal
LA English
OS CASREACT 133:30702
AB Synthesis of some new cyanopyrimido[1,2-a]pyrimidinones was achieved via interaction of 2-amino-6-anisyl-5-cyano-4(3H)-pyrimidinone with some heterocycles having a vicinal chloro ester, chlorocyano or mercaptocyano group, di-Me acetylenedicarboxylate, active methylene compds., Et 2-acetyl-3-anisylpropenoate, Et 3-aryl-3-cyanopropenoates, Et 2-cyano-3-ethoxyacrylate and some enones or enals. Some of the isolated products were subjected to biol. screening tests. This type of compound was found to be useful as co-enzymic factor in the acceleration of cellobiase activity.
IT **273940-83-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and activity of cyanopyrimido[1,2-a]pyrimidinones as cellobiase co-enzymes)
RN 273940-83-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-2-methyl-4-thioxo- (9CI) (CA INDEX NAME)



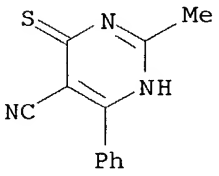

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:323074 CAPLUS
DN 127:65740
TI Synthesis of some heterobicyclic compounds bearing 4-anisyl-5-cyano-2-methyl-6-oxopyrimidin-1-yl moiety
AU Abdel-Megid, Mohamed
CS Department of Chemistry, Faculty of Education, Ain-Shams University, Cairo, Egypt
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1997), 36B(3), 269-271
CODEN: IJSBDB; ISSN: 0376-4699
PB National Institute of Science Communication
DT Journal
LA English
OS CASREACT 127:65740
AB The reactions of 4-anisyl-5-cyano-2-methyl-6(1H)-pyrimidinone I (R = H) and/or acetic acid hydrazide derivative I (R = CH2CONHNH2) with α,β-bifunctional compds., e.g., (EtO)2CHCH2Br, under different conditions have been reinvestigated and the structures of obtained heterobicyclic systems, e.g., II, were confirmed by spectroscopic methods. The mass spectra of some synthesized compds. have been studied to establish their fragmentation processes.
IT **191281-42-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyanooxopyrimidinyl heterobicyclic compds.)
RN 191281-42-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-2-methyl-4-oxo- (9CI) (CA INDEX NAME)

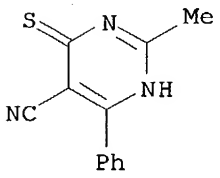



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

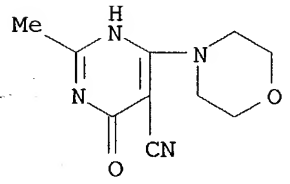
L6 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:469812 CAPLUS
DN 117:69812
TI Dimerizing condensation of alkylidenepropanedinitriles and alkylidenecyanamides. A general approach to aniline, aminopyridine, and aminopyrimidine derivatives
AU Hartke, Klaus; Sauerbier, Michaela; Richter, Wolfgang F.
CS Inst. Pharm. Chem., Univ. Marburg, Marburg, D-3550, Germany
SO Archiv der Pharmazie (Weinheim, Germany) (1992), 325(5), 279-84
CODEN: ARPMAS; ISSN: 0365-6233
DT Journal
LA German
AB The base-catalyzed dimerizing condensation of (α-methylthioalkylidene)propanedinitriles, such as MeSCMe:C(CN)2, yields 2-aminobenzene-1,3-dicarbonitriles, e.g., I; that of (α-methylthioalkylidene)cyanamides, e.g., MeSCMe:NCN, gives 2-aminopyrimidines, e.g., II. The mixed condensation of (α-aminoalkylidene)propanedinitriles,e.g., H2NCPh:C(CN)2, with (α-methylthioalkylidene)cyanamides, e.g., MeSCPh:NCN, leads to pyrimidine-5-carbonitriles, e.g., III.
IT **13996-07-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)
RN 13996-07-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-phenyl-4-thioxo- (8CI, 9CI) (CA INDEX NAME)



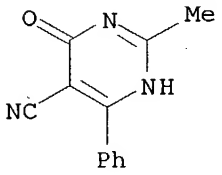
L6 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:448480 CAPLUS
DN 117:48480
TI Synthesis and biological activities of some new pyrimidine derivatives
AU Seada, M.; Abdel-Halim, A. M.; Ibrahim, S. S.; Abdel-Megid, M.
CS Fac. Educat., Ain Shams Univ., Roxy, Egypt
SO Asian Journal of Chemistry (1992), 4(3), 544-52
CODEN: AJCHEW; ISSN: 0970-7077
DT Journal
LA English
AB Synthesis of 4-chloro-5-cyano-2-methyl-6-phenylpyrimidine (I, R = Cl) and its reactions with acetamide hydrochloride, guanidine hydrochloride, cyanoacetamide, benzil monohydrazone, sodium azide, semicarbazide hydrochloride, acid hydrazides, active methylene compds., aromatic amines and thiourea were investigated. Also, the reactions of 5-cyano-2-methyl-6-phenyl-4(3H)-pyrimidinethione I (R = SH) with Et iodide, Et chloroacetate, phenacyl bromide, acrylonitrile and heterocyclic chlorides are reported. A number of products from these two series of reactions, including aminocyanopyridopyrimidinone II and (phenylbutadienyl)pyrimidine III were evaluated for bactericidal and fungicidal activity.
IT **13996-07-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of)
RN 13996-07-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-phenyl-4-thioxo- (8CI, 9CI) (CA INDEX NAME)



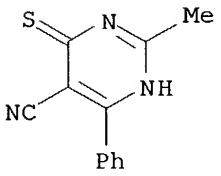
L6 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:95143 CAPLUS
DN 110:95143
TI Synthesis of pyrimidine derivatives by the reaction of ketene dithioacetals with amides
AU Kohra, Shinya; Tominaga, Yoshinori; Hosomi, Akira
CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, 852, Japan
SO Journal of Heterocyclic Chemistry (1988), 25(3), 959-68
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 110:95143
AB Reactions of Me 2-cyano-3,3-bis(methylthio)acrylate (MeS)2C:CRCN (I, R = CO2Me) with carboxamides R1CONH2(II, R1 = 4-R2C6H4, ClCH2, Me, PhCH:CH; R2 = H, NO2, Me, MeO) in the presence of NaH gave the resp. Me 3-N-acylamino-2-cyano-3-(methylthio)acrylates R1CONaC(SMe):C(CO2Me)CN, which were readily converted to the resp. pyrimidine derivs. III (R = CO2Me) at reflux in methanol in good yields. Reactions of 2-cyano-3,3-bis(methylthio)acrylonitrile I (R = CN) with the carboxamides II gave directly pyrimidine-5-carbonitrile derivs. III (R = CN). Ketene dithioacetals smoothly reacted with thioacetamide or ureas to give the expected pyrimidine derivs. Polyfunctionalized pyrimidines, thus obtained, were also used for the synthesis of fused pyrimidine derivs.
IT **118996-56-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 118996-56-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-(4-morpholinyl)-4-oxo- (9CI) (CA INDEX NAME)



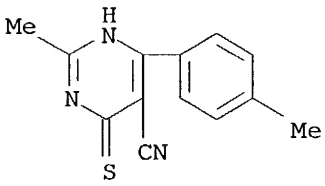
L6 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:113408 CAPLUS
DN 102:113408
TI Synthesis of 2,4-dioxo, 2-oxo-4-thioxo, 4-oxo-, and 4-thioxopyrimidine-5-carbonitriles
AU Cuadrado, Francisco J.; Perez, Miguel A.; Soto, Jose, L.
CS Dep. Quim. Org., Univ. Complutense, Madrid, Spain
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (10), 2447-9
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 102:113408
AB Cyclocondensation of Me N-methoxycarbonylimidates with NCCH2CONH2 (I) and NCCH2CSNH2 (II) in the presence of NaOMe gave tetrahydro-2,4-dioxo- and -2-oxo-4-thioxopyrimidine-5-carbonitriles, resp. E.g., 93% pyrimidinedione III (X = O) was obtained on refluxing PhCH2C(OMe):NCO2Me with I in MeOH for 12 h. Analogous reactions with alkyl N-acylimidates gave dihydro-4-oxo- and -thioxopyrimidine-5-carbonitriles. E.g., PhC(OEt):NCOC6H4Cl-4 with II gave 49% pyrimidinethione IV on refluxing for 4 h in MeOH. III (X = S) and IV were methylated to the methylthio derivs. V and VI, in 70% and 75% yield, resp., and cyclized to give 54% dihydrothienopyrimidine VII and 80% thienopyrimidine VIII, resp., on refluxing with ClCH2CO2Me and NaOMe in MeOH.
IT **82141-07-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by cyclocondensation reaction of alkyl acylimidate with cyanoacetamide)
RN 82141-07-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)



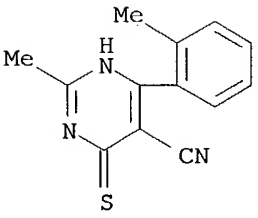
L6 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:423736 CAPLUS
DN 97:23736
TI Synthesis of heterocycles. XXI. 6-Substituted 5-cyano-2-methyl-4-pyrimidinethiones
AU Soto, Jose L.; Lorente, A.; Garcia Navio, Jose L.
CS Fac. Quim., Univ. Complutense, Madrid, Spain
SO Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1981), 77(3), 255-7
CODEN: AQSBD6; ISSN: 0211-1357
DT Journal
LA Spanish
AB Pyrimidinethiones I (R = Ph, 4-MeC6H4, 2-MeC6H4, 3-ClC6H4) were obtained in 50-75% yield by treating MeOCR:C(CN)2 with MeCSNH2. Reaction of EtOCMe:C(CN)2 with MeCSNH2 similarly gave 14% I (R = Me). I (R = Ph) was S-methylated and methylthiopyrimidine was hydrolyzed to give the pyrimidinone. KIO4 oxidation of I (R = Ph) gave the disulfide.
IT **13996-07-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 13996-07-1 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-phenyl-4-thioxo- (8CI, 9CI) (CA INDEX NAME)



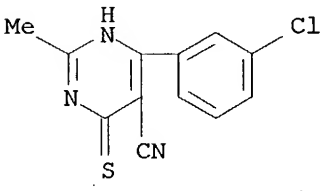

IT **82141-03-5P 82141-04-6P 82141-05-7P**
**82141-07-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82141-03-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-(4-methylphenyl)-4-thioxo- (9CI) (CA INDEX NAME)



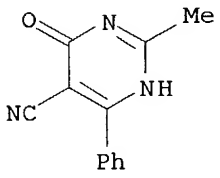

RN 82141-04-6 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-(2-methylphenyl)-4-thioxo- (9CI) (CA INDEX NAME)



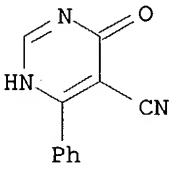
RN 82141-05-7 CAPLUS
CN 5-Pyrimidinecarbonitrile, 6-(3-chlorophenyl)-1,4-dihydro-2-methyl-4-thioxo- (9CI) (CA INDEX NAME)



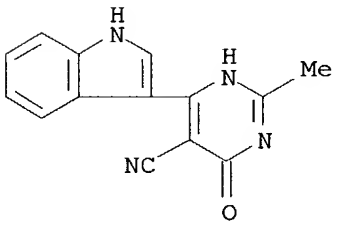
RN 82141-07-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:146395 CAPLUS
DN 92:146395
TI Syntheses with nitriles, LVII. The reactivity of aminomethylenemalonodinitriles towards aldehydes and ortho esters
AU Mittelbach, Martin; Junek, Hans
CS Inst. Org. Chem., Univ. Graz, Graz, Austria
SO Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1979), 34B(11), 1580-6
CODEN: ZNBAD2; ISSN: 0340-5087
DT Journal
LA German
OS CASREACT 92:146395
AB Condensation of H2NCH:C(CN)2 with 4-RC6H4CHO (R = Cl or NMe2) and (MeO)2CHNMe2, resp., led to 4-RC6H4CH:C(CN)2 and Me2NCH:C(CN)2, resp. A mechanism of this cleavage of a C:C double bond is discussed. Several substituted enaminonitriles H2NCR1:CR2CN (I; R1 = Me, Et or Ph; R2 = CN or CONH2) were prepared and the irreactivity against aldehydes was studied. Thus, condensation of I (R1 = Me, R2 = CN) with R3CHO (R3 = substituted Ph) gave R3CH:CHC(NH2):C(CN)2. The reaction of I (R1 = Me or Ph, R2 = CONH2) with R3CHO or CH(OEt)3 gave pyrimidinecarbonitriles II and III, resp.
IT **73249-90-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73249-90-8 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)

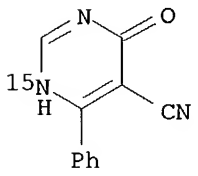


L6 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:31980 CAPLUS
DN 88:31980
TI Antitumor activity of indole derivatives
AU Kobayashi, Goro; Matsuda, Yoshiro; Tominaga, Yoshinori; Ohkuma, Mihoko; Shinoda, Hirotaka; Kohno, Morihiro; Mizuno, Den'ichi
CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SO Yakugaku Zasshi (1977), 97(9), 1033-9
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
AB Sixty-one indole derivs. containing oxindole, spiro-oxindole, and condensed-ring indole were prepared and their antitumor activity was examined using a solid type of Ehrlich carcinoma. 1-Methyl-3-(1-methylthio-1-morpholinomethylene)oxindole (I) [15127-79-4] was found to have some antitumor effect, but no other derivs. were found effective.
IT **18234-35-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antitumor activity of)
RN 18234-35-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(1H-indol-3-yl)-2-methyl-4-oxo- (9CI) (CA INDEX NAME)

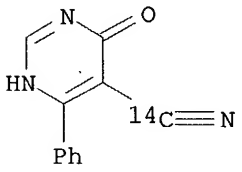


L6 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:147896 CAPLUS
DN 78:147896
TI Pyrimidines from this laboratory. XXXII. Addition nucleophile ring opening ring closing mechanism. VII. Reaction of 4-chloro-5-cyano-6-phenylpyrimidine with potassium amide in liquid ammonia at -75.deg.
AU De Valk, J.; Van der Plas, H. C.
CS Lab. Org. Chem., Agric. Univ., Wageningen, Neth.
SO Recueil des Travaux Chimiques des Pays-Bas (1973), 92(3), 471-80
CODEN: RTCPA3; ISSN: 0165-0513
DT Journal
LA English
AB By treatment with KNH2 in liquid NH3 at -75°, 4-chloro-5-cyano-6-phenylpyrimidine is converted into 4-amino-5-cyano-6-phenyl-pyrimidine; 1-amino-2,2-dicyano-1-phenylethene is formed as a minor reaction product. Evidence is presented, using the labeled compds. 4-chloro-5-cyano-6-phenyl-[1(3)-15N]- and 4-chloro-5-cyano-14C-6-phenylpyrimidine that the conversion into the corresponding 4-amino compound proceed completely according to the ANRORC mechanism, and the cyano-14C function remains nearly completely extranuclear. The synthesis of the 15N- and 14C-labeled 4-chloro-5-cyano-6-phenyl- pyrimidines is described.
IT **40889-21-2P 40889-25-6P 40904-79-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40889-21-2 CAPLUS
CN 5-Pyrimidine-1-15N-carbonitrile, 1,4-dihydro-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)

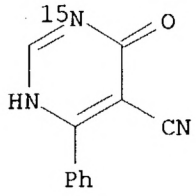
Same as # 13.



RN 40889-25-6 CAPLUS
CN 5-Pyrimidinecarbonitrile-14C, 1,4-dihydro-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)



RN 40904-79-8 CAPLUS
CN 5-Pyrimidine-1-15N-carbonitrile, 1,6-dihydro-6-oxo-4-phenyl- (9CI) (CA INDEX NAME)

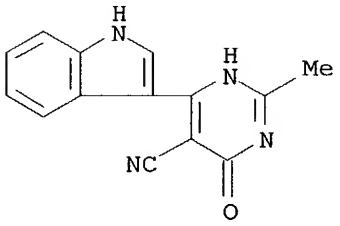

15N
O
HN
CN
Ph

L6 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:449129 CAPLUS
DN 75:49129
TI 3-Substituted indoles
IN Kobayashi, Goro; Matsuda, Yoshiro
PA Kowa Co., Ltd.
SO Jpn. Tokkyo Koho, 5 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI JP 46008698 | B4 | 19710305 | JP | 19670213 |

AB I (X and Y = CN or alkoxycarbonyl) are prepared from 2-R substituted indoles and some I are converted to II. Thus, EtMgBr was prepared from 2.3 g Mg and 10 g EtBr in 50 ml THF, treated with 10 g indole, and added to 17.4 g (MeS)2C:C(CN)CO2Me in 80 ml THF. The mixture was refluxed 1 hr to give on chromatog. 10.7 g I (R = H, X = CN, Y = CO2Me) (III), m. 145°. I prepared were (R, X, Y, and m.p. given): H, CN, CO2Et, 172°; H, CN, CN, 183-4°; H, CO2Et, CO2Et, 132°; Me, CO2Me, CO2Me, 129-32°; Me, CN, CO2Me, 152-4°; Ph, CN, CO2Me, 209-10°. Guanidine-HCl (0.17 g) and 0.04 g Na in 10 ml MeOH was clarified and refluxed 1 hr with 0.5 g III to give 0.15 g II (Z = NH2), m. >300°. II (Z = Me), m. >300°, was prepared with MeC(:NH)NH2 or NH4OAc instead of guanidine.

IT **18234-35-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18234-35-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(1H-indol-3-yl)-2-methyl-4-oxo- (9CI) (CA INDEX NAME)




Same as #14

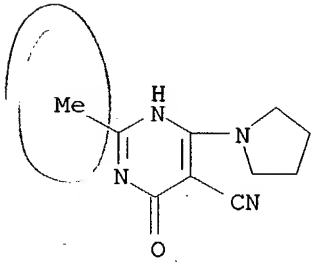
L6 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:53838 CAPLUS
DN 74:53838
TI 4-Amino-6-hydroxypyrimidines
IN Thomas, Gottfried; Braeuer, Siegfried; Fuerst, Hans; Held, Paul
SO Ger. (East), 2 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DD 72790 | | 19700505 | DD | 19681108 |

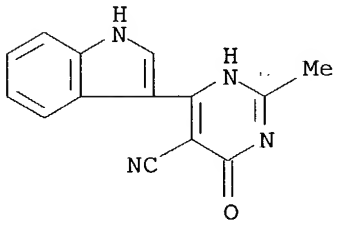
AB The title compds. (I) are obtained by treatment of a similarly substituted trichloromethylpyrimidine (II) with appropriately substituted primary or secondary aliphatic or cyclic amines R2R3NH. Thus, II (R1 = Me, Y = CO2Me) heated 20 min from 50-85° with excess H2NCH2CH2CN and the mixture treated with H2O yielded 85% I (R1 = Me, R2 = CH2CH2CN, R3 = H, Y = CO2Me), m. 278-80° (decomposition)(HCONMe2-H2O). Similarly were obtained I (R1, R2, R3, and Y given): Me, (R2R3 =) (CH2)4, CN; Ph, HOCH2CH2, H, CO2Me; Me, PhCH2, H, Bz.

IT **30393-09-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 30393-09-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 4-hydroxy-2-methyl-6-(1-pyrrolidinyl)- (8CI) (CA INDEX NAME)



L6 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:29522 CAPLUS
DN 68:29522
TI Indole derivatives. V. Reaction of 3-methylthio-3-(3-indolyl)acrylic acid derivatives with some amines
AU Kobayashi, Goro; Furukawa, Sunao; Matsuda, Yoshiro; Washida, Yuko
CS Univ. Nagasaki, Nagasaki, Japan
SO Yakugaku Zasshi (1967), 87(7), 857-60
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
AB Synthesis of I was reported. In an example, a mixture of 1 g. Me 2-cyano-3-methylthio-3-(3-indolyl)acrylate in 10 ml. MeOH is refluxed 2 hrs. with 0.45 g. ethanolamine and evaporated To the residue is added H2O, and the precipitate recrystd. from MeOH to give 90% I [R1 = NH(CH2)2OH, R2 = H, R3 = CO2Me], m. 181°. Similarly prepared are the following I (R1, R2, R3, m.p., and % yield given): pyrrolidino, H, CO2Me, 185-6°, 72; piperidino, H, CO2Me, 181°, 46; piperidino, H, H, 197°, 89; NHCH2CO2Et, H, CO2Me, 192-3°, 83; NH2, H, CO2Me, 203°, 58; NH(CH2)2OH, H, CN, 198-9°, 80; pyrrolidino, H, CN, 208°, 73; piperidino, H, CN, 221°, 70; NHCH2CO2Et, H, CN, 153°, 50; NH(CH2)2NEt2, H, CN, 153° (hydrochloride), 70; NH(CH2)2OH, Me, CO2Me, 155°, 67; NH(CH2)2NEt2, Me, CO2Me, 156°, 49; NH2, Me, CO2Me, 215°, 78.
IT **18234-35-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18234-35-0 CAPLUS
CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(1H-indol-3-yl)-2-methyl-4-oxo- (9CI) (CA INDEX NAME)




Same as #14

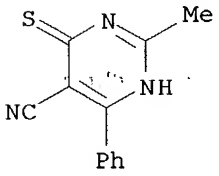
L6 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:65441 CAPLUS
DN 66:65441
TI Synthesis of pyrimidine-4-thiones and pyrazolo[3,4-d]pyrimidines
AU Goerdeler, Joachim; Wieland, Dieter
CS Univ. Bonn, Bonn, Fed. Rep. Ger.
SO Chemische Berichte (1967), 100(1), 47-59
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 66:65441
AB MeC(NH2):CHC(O)Me (I) (0.99 g.) in 15 ml. absolute Et2O was treated dropwise with 1.01 g. AcNCS in 5 ml. Et2O. The mixture was refluxed for 0.5 hr., filtered and the residue washed with absolute Et2O to yield 1.48 g. ZMe[Z = MeC(NH2):CAcC(S)NHC(O)], m. 141° (decomposition) (MeOH-petroleum ether). Similarly were prepared (% yield and m.p. given): ZEt, 73, 128°; Zpr, 72, 113°; Z-tert-Bu, 77, 129°; ZC15H31, 69, 81°; ZCH2Ph, 70, 154°; ZCH:CHPh, 68, 142°; ZC6H4OMe-p, 124°; ZC6H4Me-m, 66, 128°; ZC6H4Cl-p, 67, 157°; ZC6H4NO2-p, 85, 132°. NaSCN (1 g.) in 20 ml. absolute AcOEt and 15 ml. absolute dioxane treated with 2,3-dichloroquinazoline-7-carboxylic acid chloride at 0°, centrifuged to remove NaCl, and treated with 0.99 g. I gave 65% N-[β-amino-α-acetylthiocrotonyl]-2,3-dichloroquinazoline-7-carboxamide, m. 159° (dioxane-Et2O) (decomposition). ClCH2CH2CONCS (1.5 g.) in 5 ml. absolute Et2O were added dropwise to 1.29 g. MeC(NH2):CHCO2Et in Et2O and refluxed for 0.5 hr. to give 65% N-(β-amino-α-ethoxycarbonylthiocrotonoyl)-β-chloropropionamide, m. 125°. Similarly were prepared [% yield and m.p. (decomposition) given]: N-(β-amino-α-ethoxycarbonylthiocrotonyl)cinnamic acid amide, 77, 132°; N-(β-γ,γ-diethoxy-α-ethoxycarbonylthiocrotonoyl)benzamide, 67, -; and N-(β-amino-α-cyanothiocinnamoyl)benzamide, 49, 150°. ZMe (1 g.) in 10 ml. 2N NaOH was neutralized with 2N HCl. The solution was concentrated in vacuo and the residue was extracted with boiling ligroine to give 59% 2-MeZ', m. 149° (Z' = 4-mercapto-6-methyl-5-acetylpyrimidine). ZEt (1 g.) was kept in 10 ml. Me2CO for 5 days. The solution treated with petroleum ether gave 93% 2-EtZ', m. 154°. Similarly were prepared (% yield and m.p. given): 2-PrZ', 98, 152°; 2-tert-BuZ', 95, 156°; 2-PhCH2Z', 97, 194°; 2-PhCH:CHZ', 93, 242° (decomposition); 2-m-MeC6H4Z', 97, 184; 2-m-ClC6H4Z', 96, 217° (decomposition); 2-p-O2NC6H4Z', 98, 187° (decomposition); 4-mercapto-6-methyl-5-acetyl-2-(2-furyl)pyrimidine, 100, 185° (decomposition); 4-mercapto-6-methyl-5-acetyl-2-(3-pyridyl)pyrimidine, 64, 233°; 2-MeZ2; 92, 142° (Z2 = 4-mercapto-6-methyl-5-ethoxycarbonyl-pyrimidine); 2-PhCH:CHZ', 92, 224°; and 4-mercapto-6-diethoxymethyl-2-phenyl-5-ethoxycarbonylpyrimidine, 84, 147°. C4H9CONCS (1.43 g.) in 15 ml. EtOAc was added dropwise with stirring to 0.99 g. I in 10 ml. absolute EtOAc. The mixture was refluxed for 10 hrs. and concentrated to give 74% 2-BuZ', m. 141°. Similarly were prepared: 2-C11H23Z', m. 95°, in 70% yield and 2-C15-H31Z', m. 97°, in 84% yield. ZC6H4OMe-p (1 g.) and 1 g. anhydrous ZnCl2 in 50 ml. CH2Cl2 was shaken for 10 hrs. and evaporated in vacuo to give 82% 2-(p-C6H4OMe)Z', m. 194° (decomposition). Similarly were prepared 4-mercapto-6-methyl-5-acetyl-2-(2,3-dichloro-7-quinazolyl)pyrimidine, m. 240° (decomposition), in 84% yield, and 2-ClCH2CH2Z', m. 128°, in

78% yield. PhCH2CH2-CONCNS (1.87 g.) in 15 ml. absolute EtOAc was added dropwise to 0.99 g. I in 10 ml. absolute Et2O wtih stirring. The solution was evaporated, the residue dissolved in 2N NaOH, filtered, and extracted 2 times with
15 ml. EtOAc to give upon neutralization with concentrated HCl 78% 2-PhC.tplbond.CZ', m. 238° (AcOH-MeOH). Similarly were prepared: 1,4-bis(4-mercapto-6-methyl-5-acetyl-2-pyrimidinyl)benzene, m. 250-70° (decomposition), in 79% yield and 4-mercapto-6-phenyl-2-styryl-5-cyanopyrimidine, m. 300° (decomposition), in 69% yield. 2-C11H23Z' (1 g.) in 20 ml. 80% H3PO4 was treated with 0.7 g. NaNO2 in 10 ml. H2O under cooling to give 92% bis(6-methyl-2-undecyl-5-acetyl-4-pyrimidinyl) disulfide, m. 65° (MeOH). Similarly was prepared bis(6-phenyl-2-styryl-5-cyano-4-pyrimidinyl) disulfide, m. 253° (decomposition), in 98% yield. 2-MeZ' (1.82 g.) and 0.5 g. NaOH in 20 ml. H2O was shaken 2 hrs. with 2 g. MeI to yield 86% 4-methylthio-2,6-dimethyl-5-acetylpyrimidine, m. 47° (dioxane). Similarly were prepared 4-methylthio-6-methyl-2-phenyl-5-acetylpyrimidine, m. 68° (Me2CO), in 95% yield and 4-methylthio-6-methyl-2-phenyl-5-ethoxycarbonyl-pyrimidine, m. 51° (dioxane-H2O), in 92% yield. 2-MeZ' (1.96 g.) and 3 g. N2H4.H2O in 15 ml. EtOH was refluxed for 12 hrs. to give 92% 3,4,6-trimethylpyrazolo[3,4-d]pyrimidine (II) (R = R1 = Me), m. 208°. Similarly prepared were 3,4-dimethyl-6-phenylpyrazolo[3,4-d]pyrimidine, m. 244°, in 94% yield and 3-hydroxy-4-methyl-6-phenylpyrazolo[3,4-d]pyrimidine, m. 297°, in 72% yield.

IT **13996-07-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13996-07-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-2-methyl-6-phenyl-4-thioxo- (8CI, 9CI) (CA INDEX NAME)

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L7           0 L5

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